Space-time resolved electrokinetics in cylindrical and semi-cylindrical microchannels

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It is shown show how to employ Bessel-Fourier series in order to obtain a complete space-time resolved description of electrokinetic phenomena in cylindrical and semi-cylindrical microfluidic channels.

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The employment of Fourier series and Laplace transforms allows to solve exactly the low Reynolds number Navier-Stokes equation in rectangular microchannels [1, 2]. In Refs. [1, 2] this has been used to find the space-time resolved velocity field and current density generated by the sudden application of a possibly time dependent pressure gradient and/or an electric field. This allowed to fully characterize transient and steady state electrokinetic phenomena in rectangular microchannels. A similar characterization in the case of cylindrical and semi-cylindrical is still missing. These channel geometries (particularly the latter) are relevant for microfluidics devices fabricated from glass substrates. Typically microchannels are obtained from such substrates by means of isotropic etching which produces semi-cylindrical grooves. Here we shall show how to adapt the mathematical methods presented in Ref. [1, 2] to the cylindrical and semi-cylindrical geometries, in order to allow for a space-time resolved description of electrokinetic phenomena in these cases. The physics involved will be qualitatively the same as in the rectangular geometry, thus we will not delve into a detailed discussion, but present only the mathematical method.

Cylindrical geometry As reported before [1] the starting point for studying space-time resolved electrokinetic phenomena in microchannels is the low Reynolds number incompressible Navier-Stokes equation with a generic time and space dependent body force. The natural set of coordinates for solving this problem within cylindrical microchannels is the cylindrical coordinates (r, φ, x), where x runs along the channel axis and r, φ are polar coordinates in the channel cross-section. Using this coordinate set, the x component of the Navier-Stokes equation takes the following form

$$\frac{\partial u(r,\varphi,t)}{\partial t} - \nu \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2} \right) u(r,\varphi,t) = f(r,\varphi,t) \tag{1}$$

where u is the x component of the velocity field and f is the body force. In the case of rectangular geometry the solution of the Navier-Stokes equation was found by means of double Fourier series expansion. In other words the set of functions $\psi_{k,q} = sin\left(\frac{k\pi y}{2H}\right) sin\left(\frac{q\pi z}{2W}\right)$, $k, q \in \mathbb{N}_+$ was chosen as the appropriate complete basis set for the solution of the problem with null boundary condition over a rectangular boundary. Likewise, for a circular boundary of radius R the appropriate basis set is given by the following functions

$$\psi_{m,k}(r,\varphi) = e^{im\varphi} J_m(\alpha_{m,k} r/R) \quad m \in \mathbb{Z}, k \in \mathbb{N}_+ \tag{2}$$

The symbol J_m denotes the m^{th} Bessel function of the first kind, and $\alpha_{m,k}$ denotes its k^{th} zero. For sake of completeness let us recall that the J_m are defined as the solutions of the equations

$$\rho^2 \frac{\partial^2}{\partial \rho^2} J_m(\rho) + \rho \frac{\partial}{\partial \rho} J_m(\rho) + (\rho^2 - m^2) J_m(\rho) = 0 \tag{3}$$

and that for fixed m the following orthogonality relation exists between the functions J_m:

$$\int_0^1 d\rho \rho J_m(\alpha_{m,k}\rho) J_m(\alpha_{m,q}\rho) = \frac{1}{2}\delta_{k,q}[J_m(\alpha_{m,k})]^2 \tag{4}$$

In a similar fashion the $y_m(\varphi) = e^{im\varphi}$ are solutions of $y' = imy$ and obey the orthogonality condition:

$$\int_0^{2\pi} d\varphi y_m^*(\varphi) y_n(\varphi) = 2\pi \delta_{m,n} \tag{5}$$

where the symbol "$*$" denotes complex conjugation. Using Eq. (4) and Eq. (5), allows to normalize the basis set (2) and obtain the the following complete orthonormal basis:

$$\psi_{m,k}(r,\varphi) = \frac{e^{im\varphi} J_m(\alpha_{m,k} r/R)}{\sqrt{\pi} R J_{m+1}(\alpha_{m,k})} \quad m \in \mathbb{Z}, k \in \mathbb{N}_+ \tag{6}$$

$$\int_0^{2\pi} d\varphi \int_0^R r dr \psi_{m,k}^*(r,\varphi) \psi_{n,q}(r,\varphi) = \delta_{m,n}\delta_{k,q} \tag{7}$$

The completeness of the set (6) allows to expand the functions f and u in a double generalized Fourier series (the Bessel-Fourier series), as follows:

$$u(r,\varphi,t) = \sum_{m\in\mathbb{Z}} \sum_{k\in\mathbb{N}_+} u_{m,k}(t) \psi_{m,k}(r,\varphi) \tag{8}$$

with coefficients given by:

$$u_{m,k}(t) = \int_0^{2\pi} d\varphi \int_0^R r dr \psi^*_{m,k}(r,\varphi) u(r,\varphi,t) \quad (9)$$

Expanding the Navier-Stokes equation (1) over the basis (6) gives, thanks to the property (3) and in complete analogy with what was found previously for the rectangular geometry [1], the following set of equations:

$$\frac{\partial}{\partial t} u_{m,k}(t) + \nu \Delta^2_{m,k} u_{m,k}(t) = f_{m,k}(t) \quad (10)$$

with null-boundary condition over the $r = R$ circumference automatically fulfilled. The quantities $\Delta^2_{m,k}$, given by the following formula,

$$\Delta^2_{m,k} = \frac{\alpha^2_{m,k}}{R^2} \quad (11)$$

are, so to speak, the expansion coefficients of the Laplacian operator over the given basis set (6). The $f_{m,k}(t)$ represent the expansion coefficients of the body force f:

$$f_{m,k}(t) = \int_0^{2\pi} d\varphi \int_0^R r dr \psi^*_{m,k}(r,\varphi) f(r,\varphi,t) \quad (12)$$

If the liquid is considered as initially at rest Eq. (10) must be solved with for the initial conditions $u_{m,k}(t = 0) = 0$. Following the general line drawn in Ref. [1], the solution is easily expressed in the Laplace space as:

$$\widetilde{u}_{m,k}(s) = \frac{\widetilde{f}_{m,k}(s)}{s + \nu \Delta^2_{m,k}}. \quad (13)$$

which expresses the Laplace transform of each coefficient of the velocity profile in terms of the corresponding Laplace transformed components of the driving force. The solution $u(r,\varphi,t)$ is obtained by anti-Laplace-transform ($\mathcal{L}^{-1}$) and summing up:

$$u(r,\varphi,t) = \sum_{m\in\mathbb{Z}} \sum_{k\in\mathbb{N}_+} \mathcal{L}^{-1} \left[\frac{\widetilde{f}_{m,k}(s)}{s + \nu \Delta^2_{m,k}} \right] \psi_{m,k}(r,\varphi) \quad (14)$$

For a pressure driven flow the body force f would be given by $f(r,\varphi,t) = \frac{\Delta P(t)}{\rho L}$, with L the length of the channel, ρ the liquid density and $\Delta P(t)$ the possibly time dependent pressure difference applied at the ends of the channel. For an electro-osmotically driven flow the body force would be given by $\frac{\rho_e(r,\varphi)}{\rho} E(t)$, with $E(t)$ the applied electric field and ρ_e the electric double layer (EDL) charge density that spontaneously forms at the solid liquid interface. The latter can be found by solving the Poisson-Boltzmann equation [1] for the electric double layer potential ψ within the Debye-Hückel approximation [3]:

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2} \right) \psi(r,\varphi) = \chi^2 \psi(r,\varphi), \quad (15)$$

where χ is the inverse Debye length. Expanding over the basis (6), and using the Poisson equation $\Delta\psi = -\rho_e/\varepsilon$, like in [1] one obtains the cherge density coefficients:

$$\rho_{e(m,k)} = -\varepsilon\zeta\chi^2 \frac{\Delta^2_{m,k} I_{m,k}}{\Delta^2_{m,k} + \chi^2} \quad (16)$$

where $I_{m,k}$ denote the expansion coefficients of the unity:

$$I_{m,k}(t) = \int_0^{2\pi} d\varphi \int_0^R r dr \psi^*_{m,k}(r,\varphi). \quad (17)$$

The solution of the problem in the cylindrical geometry is formally equivalent to that of the rectangular geometry. The only difference is contained in the way the expansion coefficeint are calculated: using the double Fourier series for the rectangular case, and using the Bessel-Fourier series in the cylindrical case. Thus once the basis set appropriate for a given geometry is found, the problem is automatically solved.

Semi-cylindrical geometry In this case, the function $u(r,\varphi)$ must obey not only the condition of being null for $r = R$, but also for $\varphi = 0, \pi$. Seen in a different way, the function u must be odd under the operation $\varphi \to -\varphi$. Therefore its expansion series would contain only odd terms, i.e., it would be of the type:

$$\sum_{m\in\mathbb{Z}} \sum_{k\in\mathbb{N}_+} [\psi_{m,k}(r,\varphi) - \psi_{-m,k}(r,\varphi)] \quad (18)$$

Namely it would contain only sine terms. Therefore the orthonormal basis set suitable for the semi-cylindrical geometry is:

$$\phi_{m,k}(r,\varphi) = \frac{2\sin(m\varphi) J_m(\alpha_{m,k} r/R)}{\sqrt{\pi} R J_{m+1}(\alpha_{m,k})} \quad m,k \in \mathbb{N}_+ \quad (19)$$

Where the $\phi_{m,k}$ satisfy the orthonormality conditions:

$$\int_0^{\pi} d\varphi \int_0^R r dr \phi_{m,k}(r,\varphi) \phi_{n,q}(r,\varphi) = \delta_{m,n}\delta_{k,q} \quad (20)$$

We will write the expansion of u as:

$$u(r,\varphi,t) = \sum_{m,k\in\mathbb{N}_+} u'_{m,k}(t) \phi_{m,k}(r,\varphi) \quad (21)$$

with coefficients given by:

$$u'_{m,k}(t) = \int_0^{\pi} d\varphi \int_0^R r dr \phi_{m,k}(r,\varphi) u(r,\varphi,t) \quad (22)$$

where the prime symbol is used to distinguish these coefficients from those defined previously. Adopting the same notation for the expansion of the body force, again the expansion of the Navier-Stokes equation leads to the solution

$$\widetilde{u}'_{m,k}(s) = \frac{\widetilde{f}'_{m,k}(s)}{s + \nu \Delta^2_{m,k}}. \quad (23)$$

which is formally equivalent to Eq. (13). The charge density will be given by

$$\rho'_{e(m,k)} = -\varepsilon\zeta\chi^2 \frac{\Delta^2_{m,k} I'_{m,k}}{\Delta^2_{m,k} + \chi^2} \tag{24}$$

where

$$I'_{m,k}(t) = \int_0^\pi d\varphi \int_0^R r dr \phi_{m,k}(r,\varphi) \tag{25}$$

which is formally equivalent to Eq. (16). As an illustration of the method Fig. 1 shows a typical plot of the EDL charge density obtained from Eq. (24). All the information relevant for the description of electrokinetic phenomena in cylindrical and semi-cylindrical microchanels is contained in the coefficients $u_{m,k}, \rho_{e(m,k)}$ and $u'_{m,k}, \rho'_{e(m,k)}$, respectively. These can be used like in Ref. [1, 2] to obtain a space-time resolved description of electrokinetic phenomena. For example, for the semi-cylindrical geometry one finds the following generalized conductance matrix:

$$\mathbf{M} = \frac{1}{\rho L} \sum_{m,k} \frac{e^{-i\theta'_{m,k}(\omega)}}{\sqrt{\omega^2 + \nu^2 \Delta^4_{m,k}}} \mathbf{A'}_{m,k} \tag{26}$$

Where L is the channels's length, ω is the angular frequency of the driving body force,

$$\mathbf{A'}_{m,k} \doteq \begin{pmatrix} I'^2_{m,k} & I'_{m,k}\rho'_{e(k,q)} \\ I'_{m,k}\rho'_{e(k,q)} & \rho'^2_{e(k,q)} \end{pmatrix} \tag{27}$$

and

$$\theta'_{m,k}(\omega) = \arctan\left(\frac{\omega}{\nu \Delta^2_{m,k}}\right). \tag{28}$$

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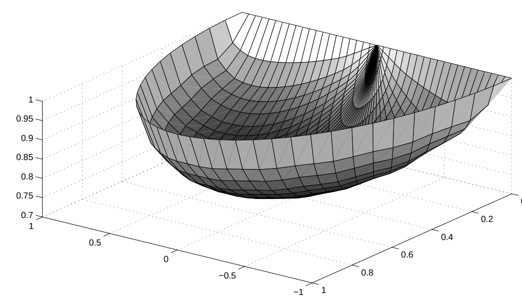

FIG. 1: Typical EDL charge density profile in non-dimensional units ($R = 1, \rho_e(1,\phi) = 1$). The first 100×100 Bessel-Fourier coefficients have been employed to generate the plot.